

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 2.67e-02 mol/L

**Global applicability domain:** Outside

**Local applicability domain index:** 2.26e-01

**Confidence level:** 4.74e-01

## Nearest Neighbors from the Training Set

Image not found

Sulfaguanidine

**Measured:** 1.03e-02

**Predicted:** 4.21e-02

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Aziprotryne

**Measured:** 2.44e-04

**Predicted:** 1.08e-02

Image not found

Arginine

**Measured:** 1.04

**Predicted:** 7.61e-01

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Azidamfenicol [INN:BAN:DCF]

**Measured:** 6.77e-02

**Predicted:** 4.38e-02